

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 290 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.11e-01

Confidence level: 8.08e-01

Nearest Neighbors from the Training Set

Image not found

4-Aminoazobenzene

Measured: 617

Predicted: 438

Image not found

N-Pentyl N-phenylcarbamate

Measured: 407

Predicted: 375

Image not found

Chlorbufam

Measured: 162

Predicted: 235